Heptane

142-82-5 | DTXSID6024127

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 231

Global applicability domain: Inside

Local applicability domain index: 6.02e-01

Confidence level: 7.26e-01

Nearest Neighbors from the Training Set

Image not found
Cyclohexane
Measured: 83.2
Predicted: 59.1

Image not found
Methylcyclohexane
Measured: 186
Predicted: 233

Image not found
Dibenzofuran
Measured: 1510
Predicted: 14.2

Image not found
Carbazole
Measured: 170
Predicted: 10.1

Image not found
1-Methoxynaphthalene
Measured: 162
Predicted: 11.2